

## PhD and Postdoc Positions in Theoretical Chemistry at the University of Fribourg, Switzerland

*Join us in shaping the future of quantum chemistry and materials science!*

I am looking for highly motivated researchers to join my **Theoretical Chemistry Group** at the University of Fribourg. We currently have **two fully funded PhD positions** and **one postdoctoral position**, supported by an **ERC Starting Grant** and the **Swiss National Science Foundation (SNSF)**. My dynamic group ([www.stefanvuckovic.com](http://www.stefanvuckovic.com)) works at the interface of **quantum chemistry and machine learning**, developing **next-generation density functional theory (DFT) methods** to tackle long-standing challenges such as **strong electronic correlation** and the **accurate description of noncovalent interactions**. Check out our recent publications (<https://www.stefanvuckovic.com/publications>) to get familiar with our work.

Successful applicants will contribute to a project based on a **new paradigm for constructing next-generation DFT methods**, with the goal of advancing the treatment of strong correlation and noncovalent interactions and applying these methods to **challenging catalysts, metal–organic frameworks, and metalloenzymes**. We are based in the **Department of Chemistry at the University of Fribourg (UNIFR)**, located in the bilingual city of Fribourg, where the French- and German-speaking parts of Switzerland meet. The city is well connected, only **20 minutes by train from Bern** and **40 minutes from Lausanne**, while offering a **lower cost of living (e.g., housing)** compared to its neighboring cities.

**Postdoctoral Position.** We are seeking a researcher with a PhD in chemistry, physics, computational science, or a related field who can work independently at the interface of **machine learning and quantum chemistry**. Candidates should have strong expertise in at least one of the following areas (more than one is a strong advantage): (1) machine learning practices (e.g., PyTorch implementations); (2) development and implementation of quantum-chemistry methods (DFT or wave-function based); (3) high-level electronic-structure calculations for generating training data (e.g., CASSCF, CASPT2, FCI).

**PhD Positions.** We are looking for motivated candidates with a Master's degree in chemistry, physics, or a related field who are eager to learn both **quantum chemistry and machine learning**. Coding skills (e.g., Python) and prior experience in computational/theoretical chemistry or machine learning are desirable. PhD positions are **fully funded**, with a typical trajectory of about **4 years** in our group.

### We offer:

- Fully funded positions (ERC/SNSF) with excellent working conditions (salary and project resources).
- A stimulating, supportive, and interdisciplinary work environment.
- Personal mentoring and guidance to maximize your career development.

UNIFR is close to the CECAM headquarters in Lausanne, where multiple workshops and schools in our field are held every year, providing further opportunities for networking.

**Start date.** Preferred **November 2025**, with flexibility.

**How to apply.** Please send **one PDF** containing: (1) your CV; (2) a brief cover letter (previous experience + motivation); and (3) the names of **two referees** to [stefan.vuckovic@unifr.ch](mailto:stefan.vuckovic@unifr.ch).